

Effect of alloying additions on twinning in Ni-based superalloys

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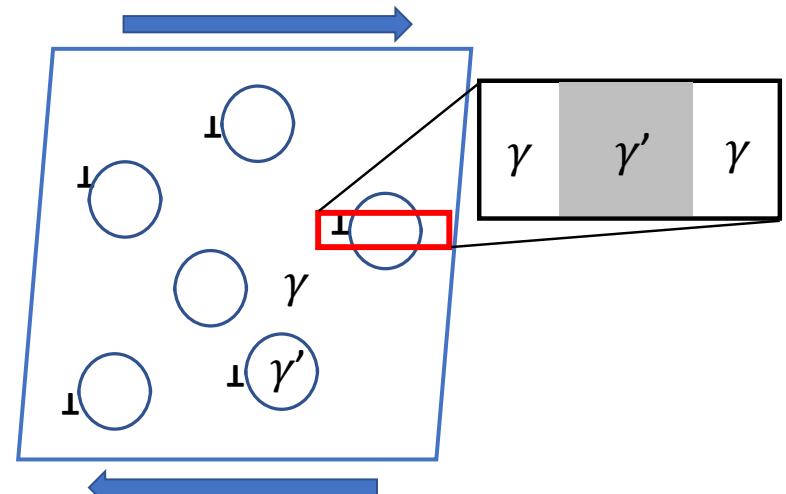
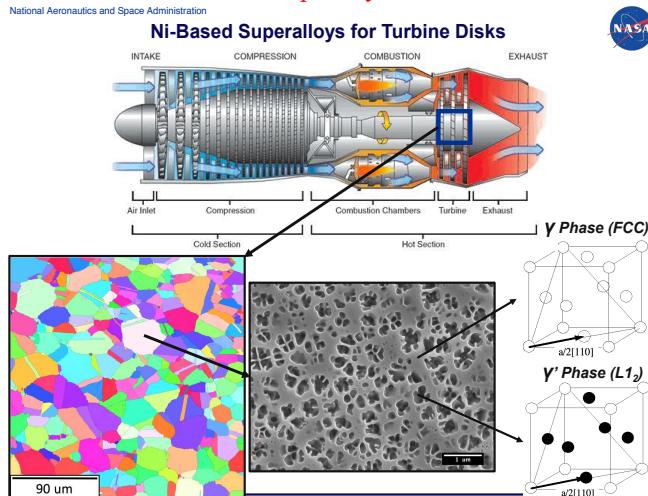
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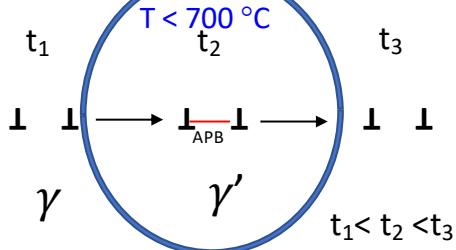


Deformation mechanisms in Ni-based superalloys

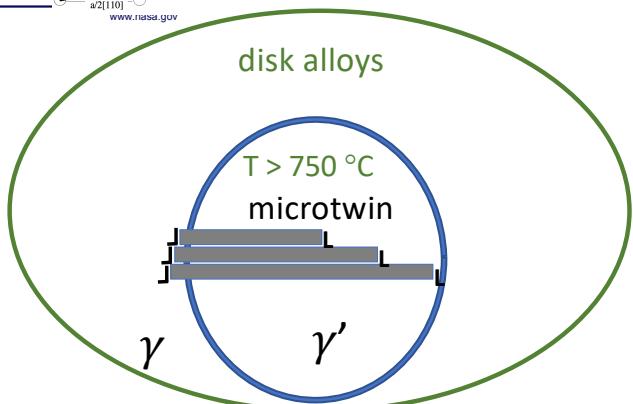
NASA report by T. Smith



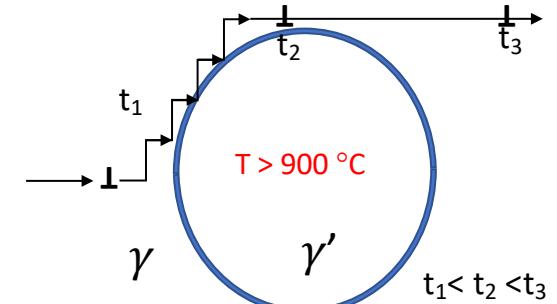
disk alloys



disk alloys

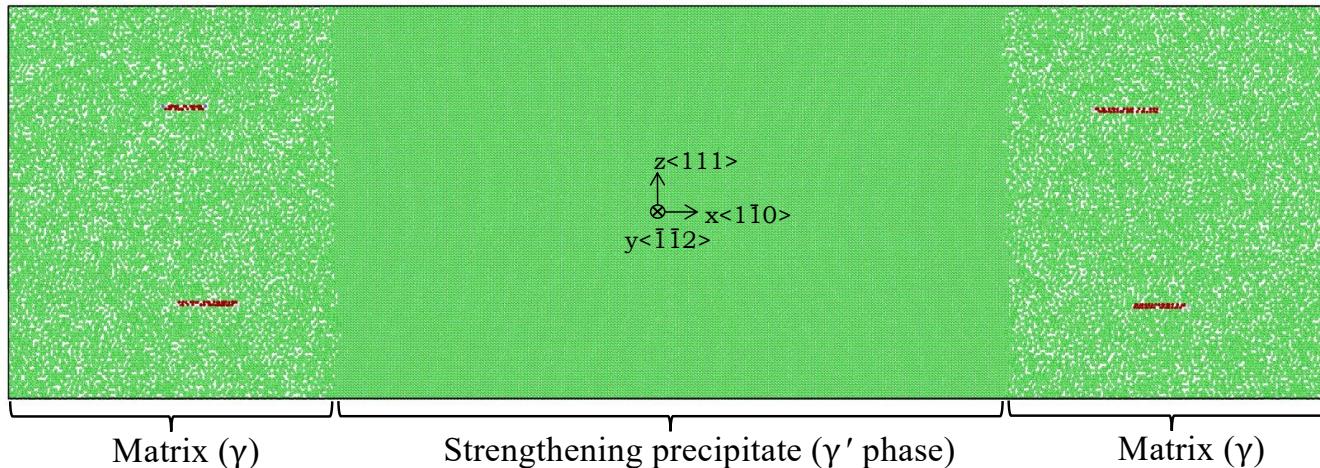


blade alloys



Simulation geometry and procedure

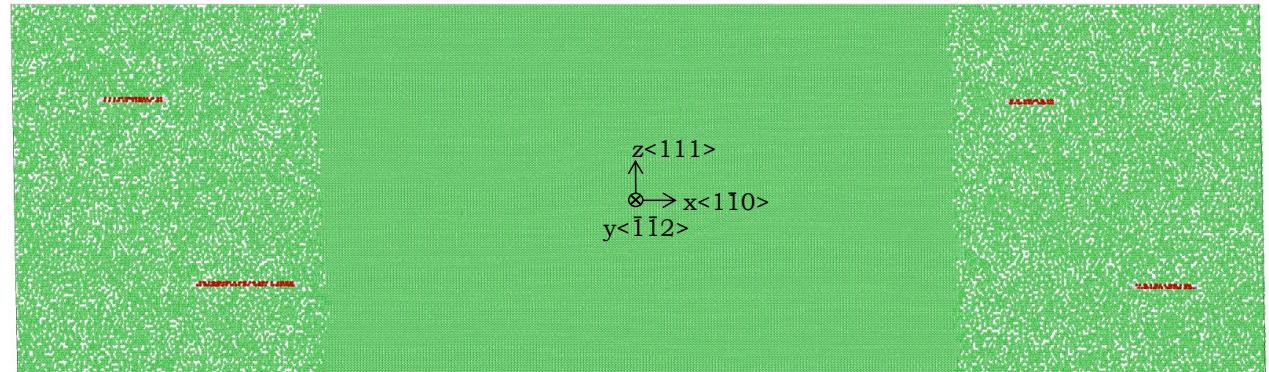
- Composite simulation system (Ni-Al), containing γ phase (matrix) and γ' phase (precipitate) regions and two edge dislocation dipoles.
- LAMMPS package; Ni-Al interatomic potential by Mendelev.
- Simulation cell size: $\sim 100 \times 2.5 \times 30 \text{ nm}^3$ ($\sim 7 \times 10^5$ atoms). PBCs in all directions.
- The system was equilibrated at $T = 1000\text{K}$, using hybrid MC/MD prior to introduction of dipoles.
- The dipoles were positioned in such a way that individual dislocations of upper and lower dislocation pairs would glide on adjacent $\{111\}$ planes when a shear stress was applied.



Two deformation modes

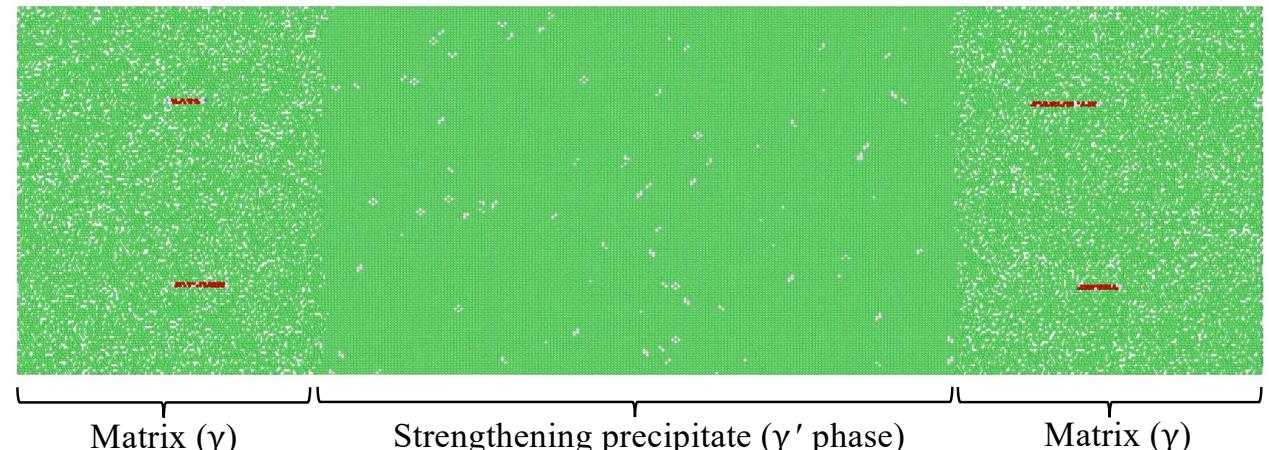
- Applied σ_{xz} shear stress: **full dislocations** interact with precipitate

New mechanism



- Applied $\sigma_{xz} + \sigma_{yz}$ shear stress: **dissociated dislocations** interact with precipitate

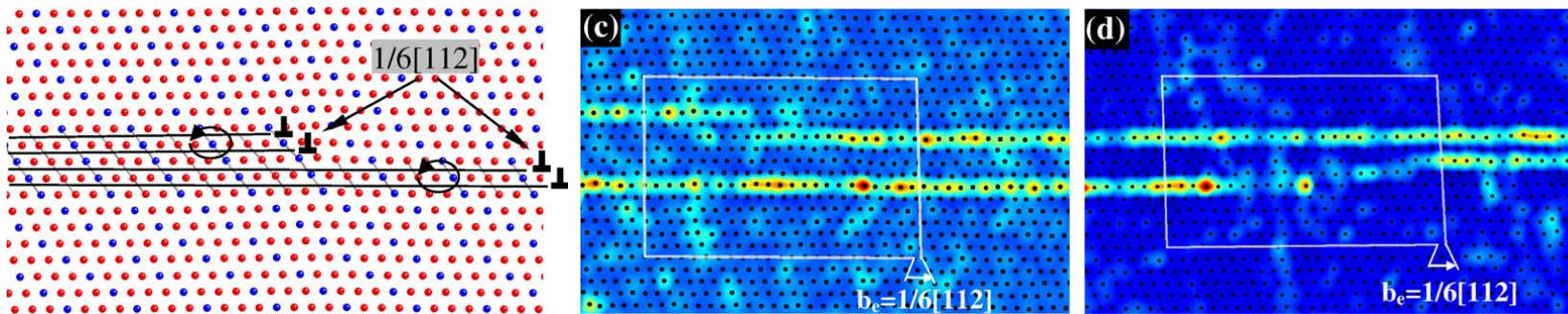
The Kolbe mechanism



The Kolbe mechanism for micro-twinning

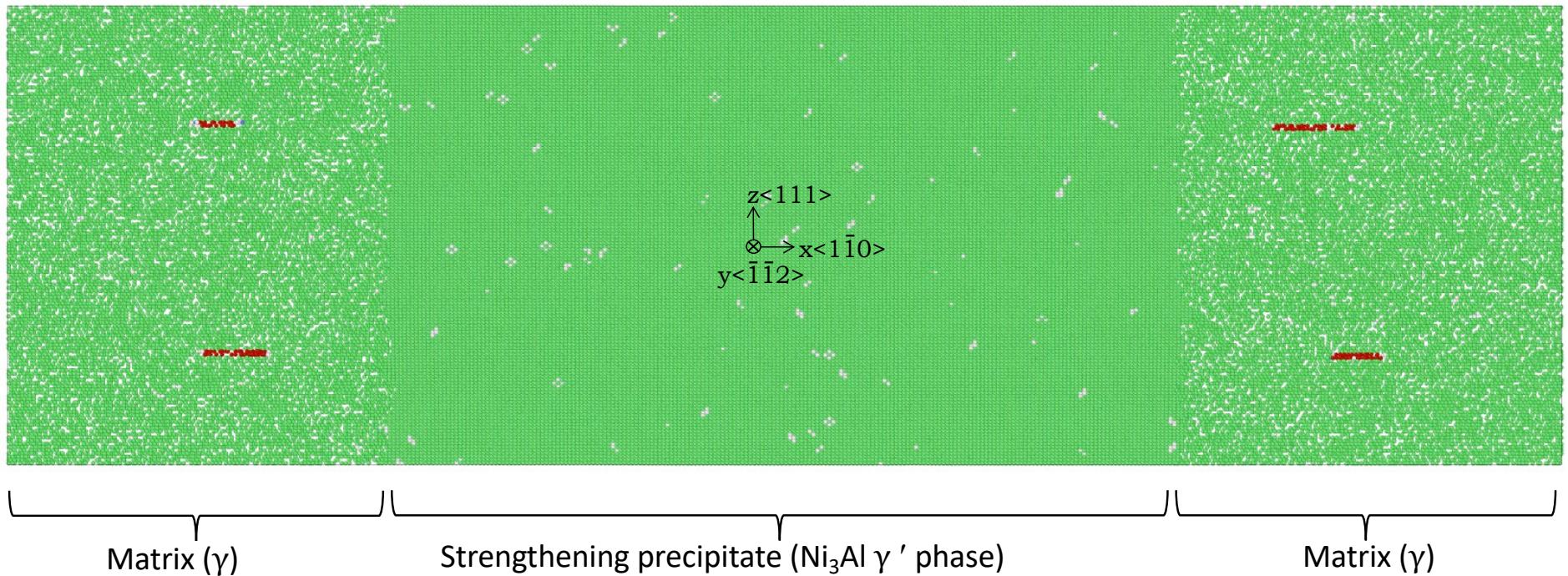
- Micro-twinning is a dominant creep deformation mechanism in Ni-based superalloys at intermediate temperatures.
- Many aspects of twin nucleation and growth remain unexplored.
- The Kolbe mechanism for micro-twinning, based on thermally activated reordering, is currently widely accepted in the community to explain these processes.

Kovarik *et al.*, PMS 2009

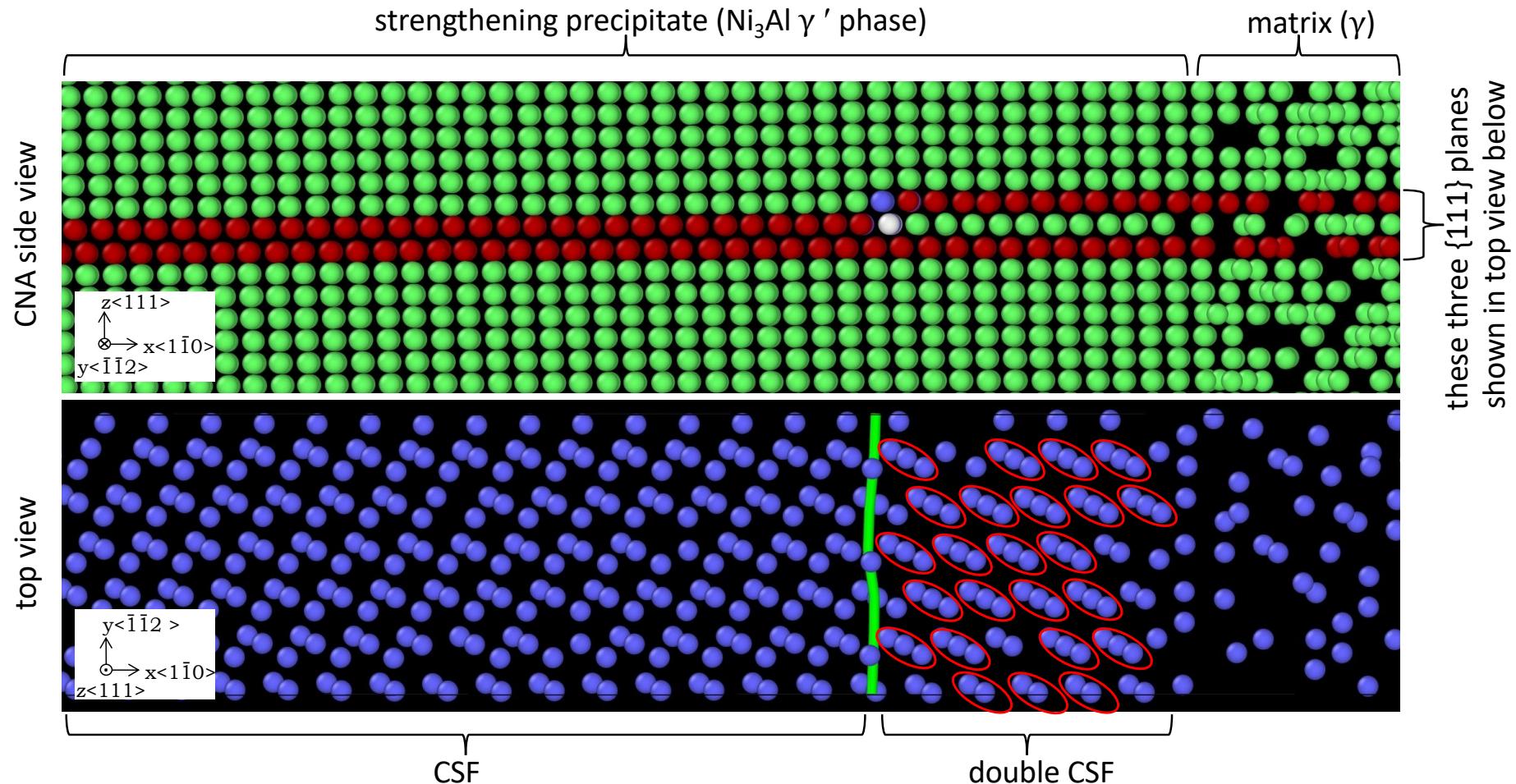


The Kolbe mechanism for micro-twinning

potential for NiAl by Mendelev; NPT, T=1300K; 350 vacancies; $\sigma_{xz} = 600$ Mpa, $\sigma_{yz} = 1039$ Mpa; Ni atoms not shown

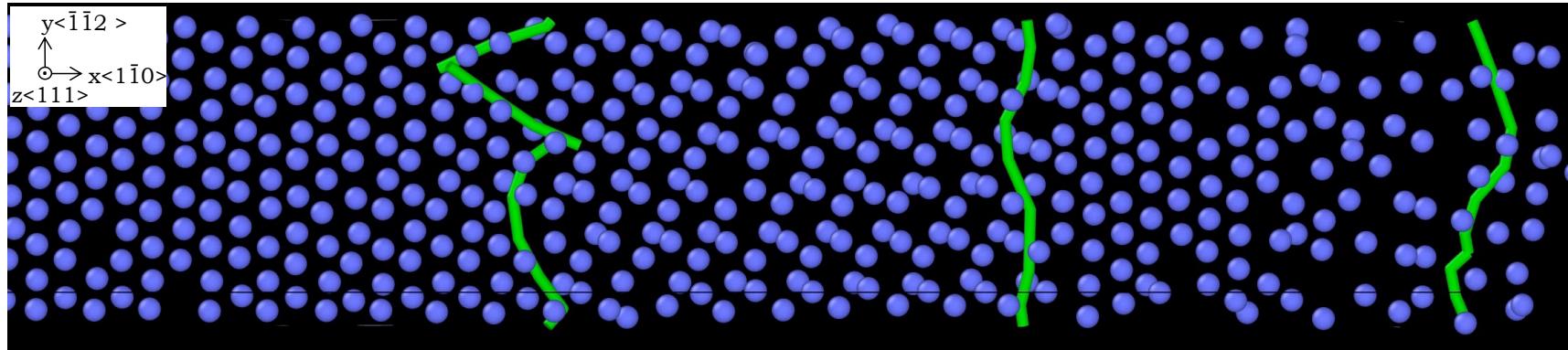


The Kolbe mechanism for micro-twinning

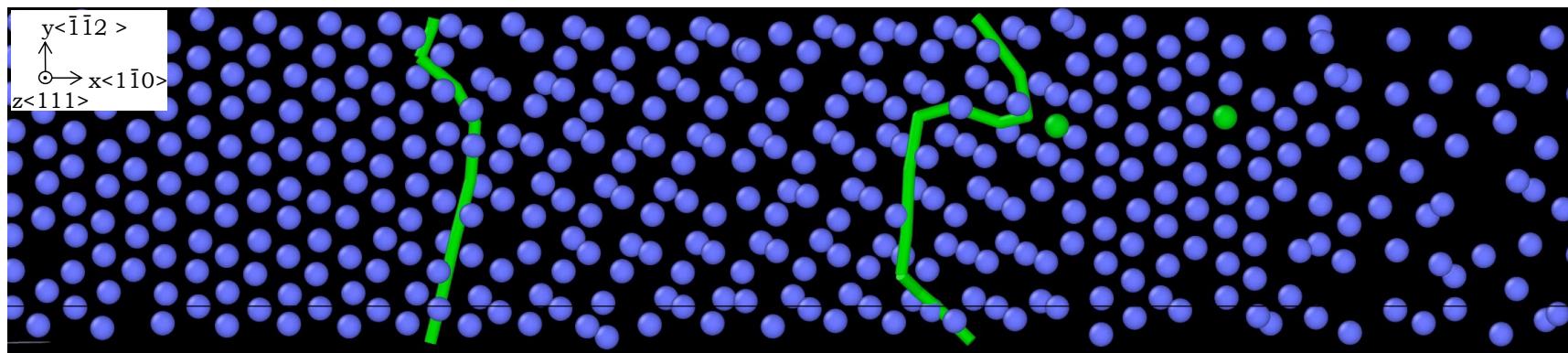


The Kolbe mechanism for micro-twinning

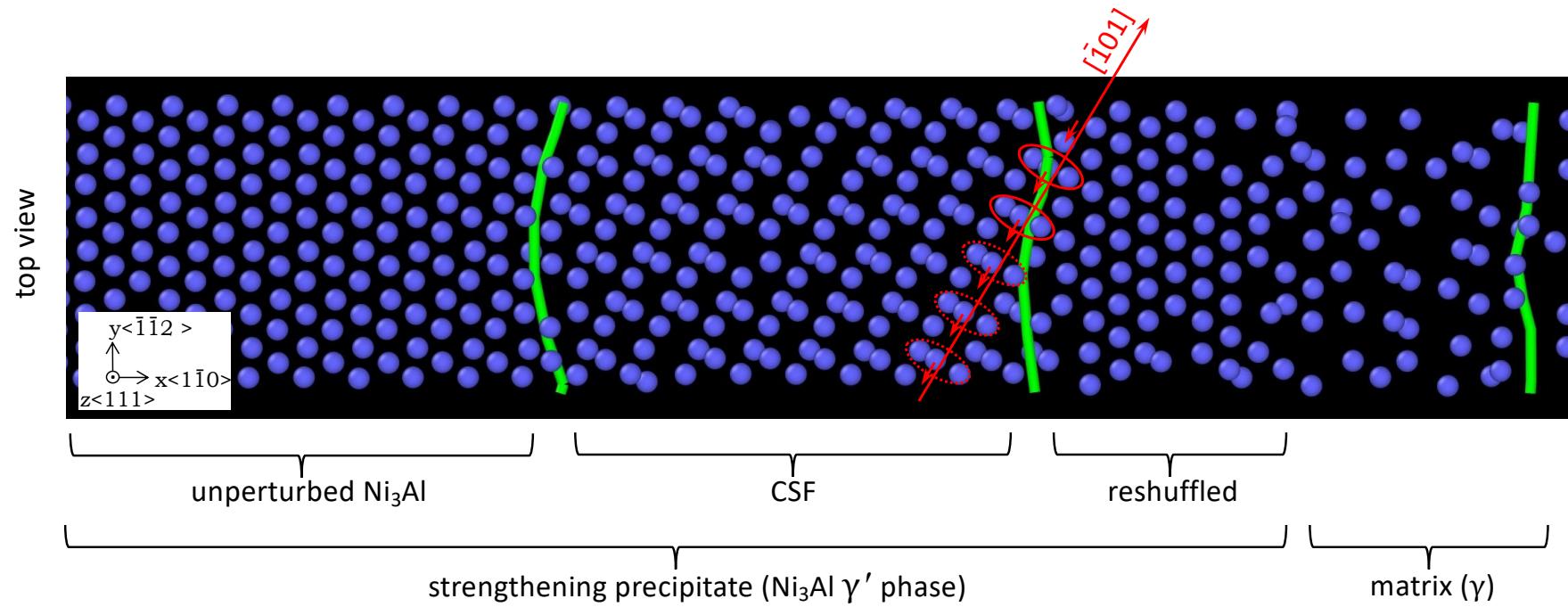
~0.1 μ s of MD deformation run (350 vacancies, T=1300K, $\sigma_{xz} = 600$ MPa $\sigma_{yz} = 1039$ MPa), Ni not shown



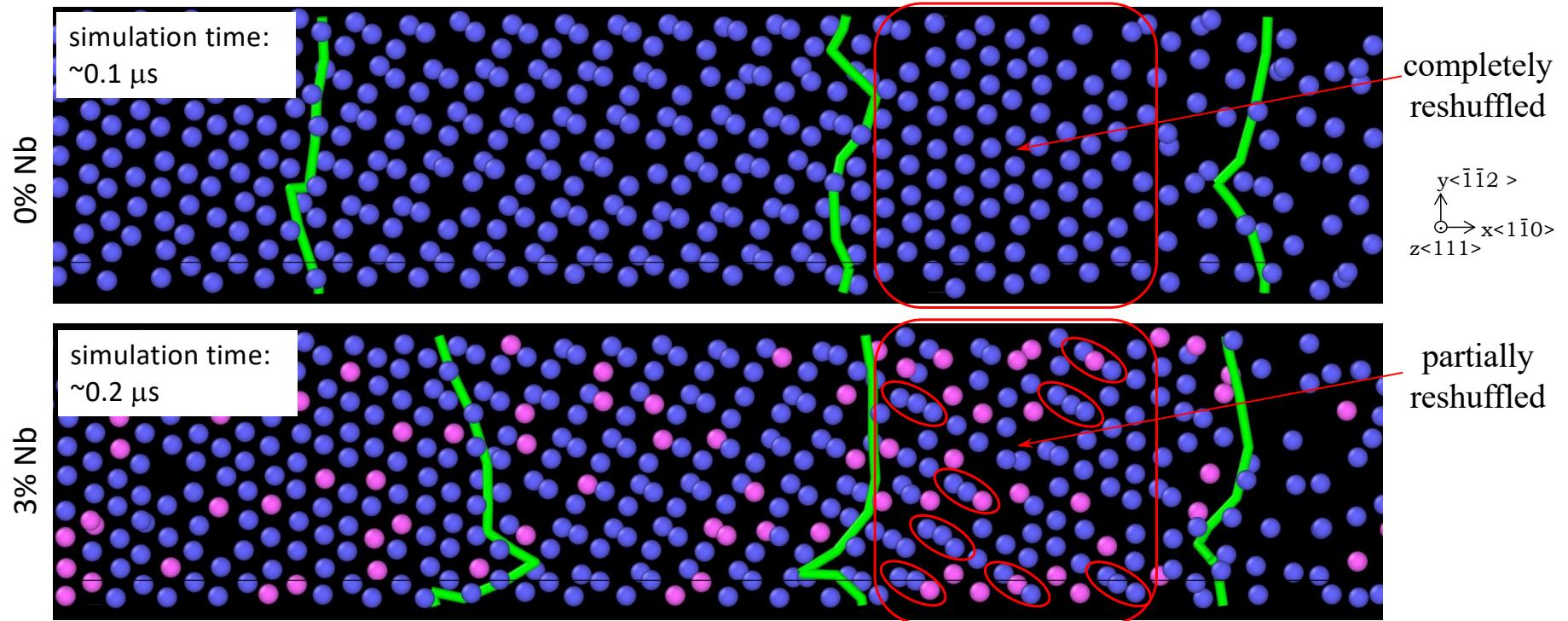
Single reshuffling move assisted by partial (vacancies are shown, Ni not shown)



The Kolbe mechanism for micro-twinning



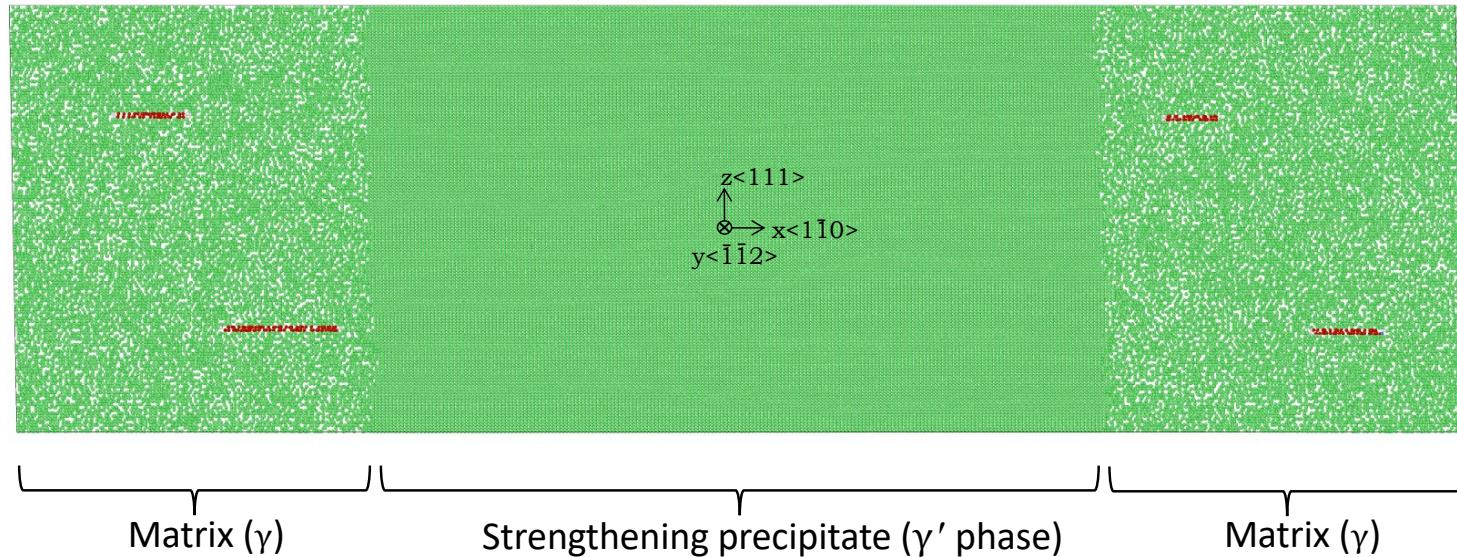
Effect of Nb on the Kolbe mechanism for micro-twinning potential for Ni-Al-Nb by Mendelev; dislocations (green); Ni atoms are not shown



- Nb atoms slow down reshuffling process. This leads to suppression of the deformation creep.

New twin nucleation and growth mechanism

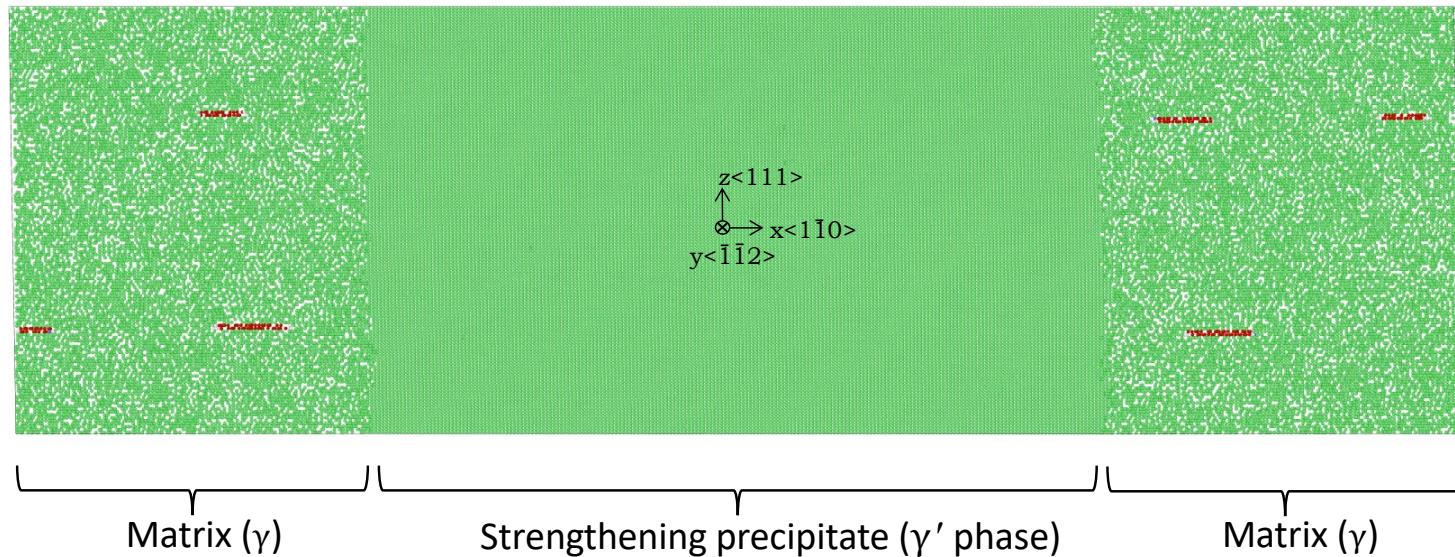
potential for NiAl by Mendelev; NPT, T=1000K; $\sigma_{xz} = 800$ Mpa; Ni atoms are not shown



- The first step of twin nucleation and growth is formation of SISF inside precipitate.

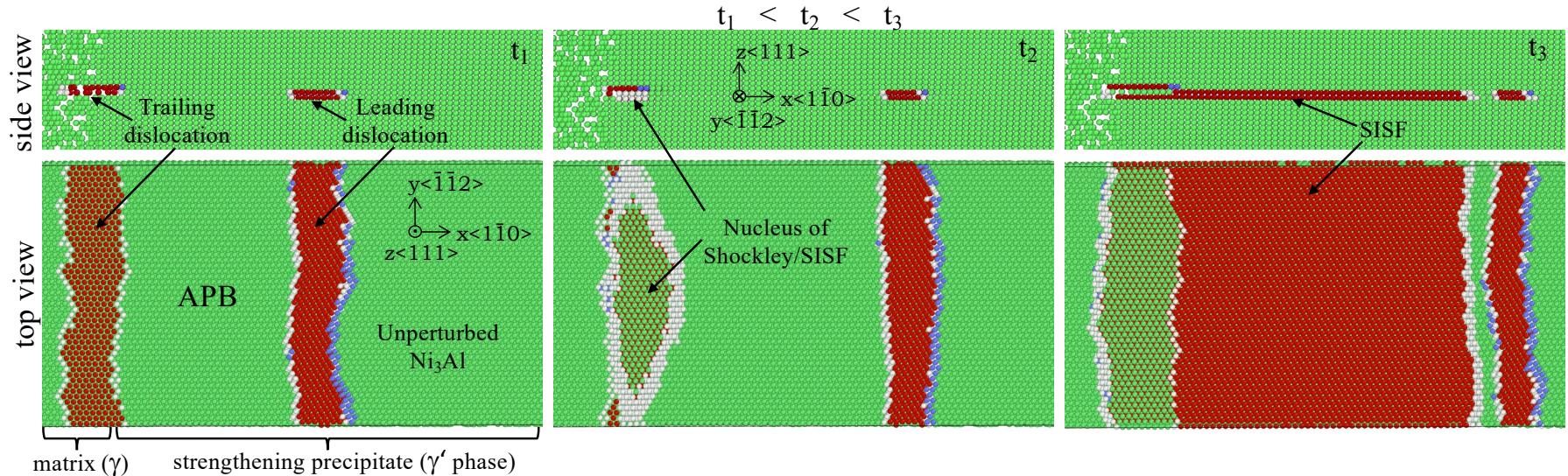
New twin nucleation and growth mechanism

potential for NiAl by Mendelev; NPT, T=1000K; $\sigma_{xz} = 800$ Mpa; Ni atoms are not shown



- The second step of twin nucleation and growth is formation of SESF inside precipitate.
- Recurring arrival of additional lattice dislocations from γ matrix will lead to growth of twin.

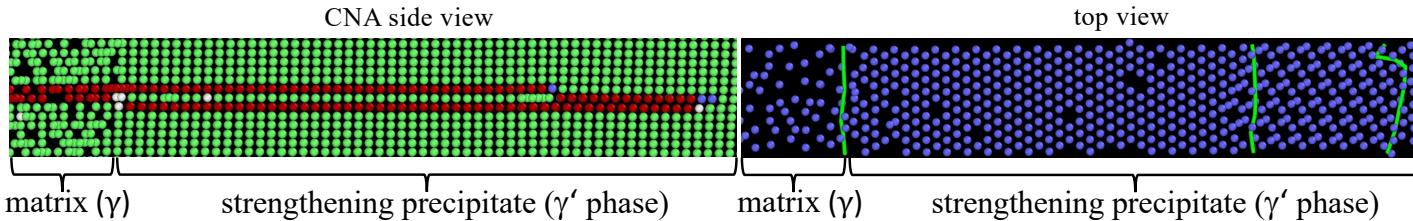
New twin nucleation and growth mechanism



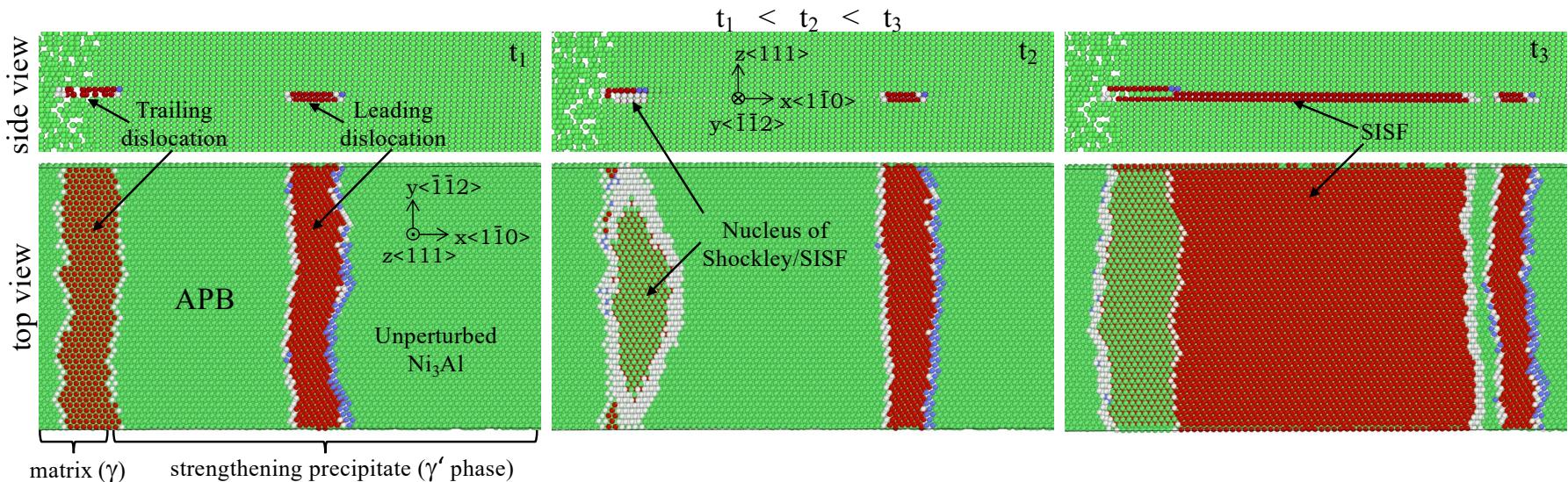
- In pure Ni-Al the new mechanism operates under applied shear stress $\sigma_{xz} > 700$ MPa (critical stress).
- Addition of 3%Nb increases the critical stress σ_{xz} up to 1.1 GPa ($\sim 50\%$ increase).
- Nb atoms suppress the process of Shockley partial nucleation.

Comparing two mechanisms

- In the Kolbe mechanism twin can grow due to passage of two Shockley partials that create 2-layer CSF that can be reordered. The process adds two layers to the twinned structure. The reordering is the rate limiting process. Nb solutes slow down reordering.



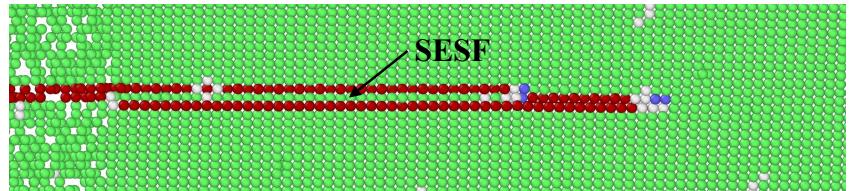
- In the proposed mechanism reordering is not involved. Single step adds one layer. The rate limiting process is nucleation of Shockley partial. Nb solutes slow down the process of nucleation of Shockley partial.



Conclusions

- Two qualitatively different mechanisms of twin growth in Ni-superalloys.
- The rate-limiting process in the Kolbe mechanism is thermally activated reordering (via vacancy diffusion).
- The rate-limiting process of the new mechanism is nucleation of the Shockley partial.
- Our results demonstrate that it is possible to neutralize multiple creep deformation mechanisms using a single solute addition.

The Kolbe mechanism



The new mechanism

